

L-Phenylalanine, N-benzoyl-

Other names:	N-Benzoyl-L-phenylalanine Benzoyl-L-phenylalanine L-BPA N-Benzoylphenylalanine, L- (2S)-2-(Benzoylamino)-3-phenylpropanoic acid
Inchi:	InChI=1S/C16H15NO3/c18-15(13-9-5-2-6-10-13)17-14(16(19)20)11-12-7-3-1-4-8-12/h1-
InchiKey:	NPKISZUVEBESJI-AWEZLNQCLSA-N
Formula:	C16H15NO3
SMILES:	O=C(NC(Cc1ccccc1)C(=O)O)c1ccccc1
Mol. weight [g/mol]:	269.30
CAS:	2566-22-5

Physical Properties

Property code	Value	Unit	Source
chs	-7941.40	kJ/mol	NIST Webbook
gf	0.95	kJ/mol	Joback Method
hf	-229.71	kJ/mol	Joback Method
hfus	34.14	kJ/mol	Joback Method
hvap	91.98	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.112		Crippen Method
mcvol	207.770	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	868.49	K	Joback Method
tc	1096.36	K	Joback Method
tf	521.26	K	Joback Method
vc	0.775	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.70	J/molxK	868.49	Joback Method
cpg	619.38	J/molxK	906.47	Joback Method
cpg	629.13	J/molxK	944.45	Joback Method

cpg	638.02	J/mol×K	982.43	Joback Method
cpg	646.14	J/mol×K	1020.40	Joback Method
cpg	653.55	J/mol×K	1058.38	Joback Method
cpg	660.33	J/mol×K	1096.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2566225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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